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This report represents the conclusion of an extensive effort comparing VIM and MC^2-2 calculations for infinite homogeneous media, evaluating observed differences in broad-group calculations, examining the corresponding algorithms for cross-section preparation and usage, and developing and/or implementing improved methods where practical.

In the first chapter, "Cross Section Preparation for the Continuous-Energy Monte Carlo Code VIM," the improvements made in the VIM library processing system are outlined. The effect of the improved methods is demonstrated through the comparison of VIM and ETØE-2/MC^2-2 calculations of broad-group cross sections for infinitely dilute materials in infinite homogeneous media. In the second chapter, "A Comparison of VIM and MC^2-2 — Two Detailed Solutions of the Neutron Slowing-Down Problems," the VIM and MC^2-2 comparison is carried on to an infinite, homogeneous core composition representative of the benchmark ZPR-6 Assembly 7. The good agreement observed again demonstrates the success of the improvements implemented. The sources of the few remaining differences observed in the reported calculations are examined.

The report illustrates the final stage of treatment of ENDF/B Version 3 data; the experience gained has resulted in further improvements being made in the treatment of ENDF/B Version 4 cross section data by the two code systems. Although the representation and usage of cross section data by VIM and by ETØE-2/MC^2-2 are extremely dissimilar, the comparison of solutions of fundamental mode slowing-down problems by VIM and by MC^2-2 has led to improvement in both codes. Furthermore, the extremely good agreement which has been demonstrated suggests that either code provides a reliable computational benchmark capability.

Chapter 1

CROSS SECTION PREPARATION FOR THE CONTINUOUS-ENERGY MONTE CARLO CODE VIM

Improvements in the methods used to represent cross sections in the data library for the Monte Carlo code VIM are discussed. The degree to which observed difficulties have been eliminated and the reliability of the current VIM library based on ENDF/B Version 3 data are illustrated by comparison of broad-group cross section calculations made by VIM and by ETØE-2/MC^2-2.

(Monte Carlo, cross section, resonance, unresolved, probability, thinning, interpolation)

Introduction

The continuous-energy Monte Carlo code VIM is in active use at Argonne National Laboratory for the analysis of fast critical experiments.[1] Through the use of large point microscopic cross section sets, VIM is intended to provide an accurate representation of neutron physics as derived from ENDF/B data. Consequently, an intensive effort has been made to identify and resolve significant discrepancies which in the past have been observed in comparisons of broad-group cross section and reaction rate calculations made by VIM and by ETØE-2/MC^2-2.[2] In the discussion following, the difficulties observed and the solutions implemented will be examined. Examples will be presented which demonstrate the degree of consistency which has been obtained by the numerous refinements made to the VIM cross section library preparation system and to ETØE-2/MC^2-2. A detailed comparison of a VIM calculation with an ETØE-2/MC^2-2 calculation using the improved capabilities is presented in a companion paper.[3]

The VIM Cross Section Library Preparation System

The VIM cross section library system is based on five codes originally developed by Atomics International. The VIMB3 code produces a BCD library from ENDF/B Version 3, reformatting the data to the needs of the other codes and reconstructing ENDF/B File 3, 4, and 5 data into formats to be used in VIM. The UNIDØP-THIN code (a descendent of UNICØRN)[4] constructs a Doppler-broadened cross section set from resonance parameters, merges it with File 3 data, and thins the output set to an interpolation error criterion. U3R produces unresolved resonance probability tables from ENDF/B unresolved resonance parameters;[5] recent extensive modifications have produced a descendent of U3R, called AURØX, which is being used for current processing of Version 4 data. The REDUCE code is used to contract the size of probability tables from a U3R or AURØX library to a desired size for VIM use. VIMTAP merges the output of VIMB3, UNIDØP-THIN, and REDUCE into a single isotopic cross section data file as used in the VIM Monte Carlo code.

All of the above codes have undergone considerable development at Argonne with respects to increased flexibility and efficiency. A major factor has been the implementation of dynamic storage allocation[6] to permit the generation of very large point data sets.

Resolved Resonance Methods

In comparison of VIM calculations with ETØE-2/MC^2-2 calculations, large local discrepancies in resolved resonance broad-group cross section output were detected. The source of the difficulties was traced to the following:

(1) insufficient point densities away from resonance peaks in the VIM and ETØE-2 libraries;

(2) failure to sum all resonance contributions at each grid point in UNIDØP and ETØE-2 (a feature optionally available with the MC^2-2 integral transport method for heavy resonance isotopes); and

(3) failure of the UNIDØP thinning method to prevent large relative distortion of absorption cross sections in the valleys between well-separated resonances.

To eliminate the first difficulty, a new algorithm to determine energy grid spacing relative to a single resonance was developed. The new algorith, based on the assumption of linear-linear cross section versus energy interpolation, replaces Otter's algorithm[4] which assumed log-linear interpolation. The new method, more consistent with actual VIM cross section usage, provides a greater relative point density in the wings of resonances than the original algorithm. Typically, 97 points per s-wave resonance and 47 or more points per p-wave resonance have been used. The code supplements the points generated around resonances with a 10-point per decade base energy grid. In the preparation of the final VIM Version 3 library, some inadequacy in grid point density between isolated resonances remained, as will be demonstated below.

An option to sum all resonance contributions at each energy point was incorporated in UNIDØP-THIN and has been employed in all cross section sets created for VIM at Argonne. Many large observed discrepancies, particularly in low energy scattering, have been eliminated by this step.

The original thinning procedure developed at Atomics International for use with UNIDØP was based only on accuracy of interpolating on total cross section. The method employs a "look ahead" procedure, extrapolating from an adjacent pair of points on the total cross section versus energy grid to find the last of a sequence of points, all of which lie within an input criterion of the extrapolation line. The first and last points of the sequence are retained and the intermediate points eliminated from the grid. The accuracy for interpolation on the thinned grid becomes a function of the cross section values over the region, but it may be shown that as the fractional error input criterion becomes small, the fractional interpolation error is bounded by approximately twice the input criterion.

The disadvantage encountered in the original application was the significant loss of accuracy in representing absorption cross sections away from resonance peaks. To obtain thinned resonance cross section of more uniform accuracy, the original algorithm is now applied twice, first to the total cross section and then to the absorption cross section, and points are thinned out of the grid only if both accuracy criteria are satisfied. In practice, a more restrictive criterion is applied to interpolation on total cross section, maintaining high accuracy in regions of greatest

TABLE II. Comparison of Infinite Dilution Broad-Group Resonance Cross Sections for Structural Materials and ^{23}Na

	Cr σ_c		Ni σ_c		Fe σ_c	
Group	MC^2-2	VIM/MC^2-2	MC^2-2	VIM/MC^2-2	MC^2-2	VIM/MC^2-2
6	0.00389	1.067 ± 0.004	0.00755	1.005 ± 0.001	0.00514	1.000 ± 0.001
7	0.00394	1.012 ± 0.008	0.00793	1.006 ± 0.003	0.00498	1.000 ± 0.001
8	0.00396	1.005 ± 0.020	0.00962	1.004 ± 0.005	0.00611	1.000 ± 0.001
9	0.00670	1.014 ± 0.028	0.01400	0.996 ± 0.005	0.00549	1.000 ± 0.001
10	0.00976	1.017 ± 0.022	0.01706	1.005 ± 0.006	0.00876	1.000 ± 0.001
11	0.01532	1.035 ± 0.036	0.0227	0.996 ± 0.033	0.00757	1.029 ± 0.089
12	0.0314	1.055 ± 0.040	0.0404	1.002 ± 0.051	0.0212	0.995 ± 0.055
13	0.0335	1.040 ± 0.061	0.0667	1.010 ± 0.023	0.00519	0.963 ± 0.148
14	0.0318	1.000 ± 0.007	0.1002	1.012 ± 0.038	0.00989	1.050 ± 0.078
15	0.0853	1.000 ± 0.004	0.0200	1.012 ± 0.029	0.0271	1.007 ± 0.010
16	0.0641	1.003 ± 0.002	0.0350	1.001 ± 0.014	0.00790	1.001 ± 0.008
17	0.0254	1.000 ± 0.001	0.0487	0.984 ± 0.060	0.00542	1.012 ± 0.015
18	0.2236	1.079 ± 0.076	0.0224	1.003 ± 0.007	0.01114	1.097 ± 0.030
19	0.01982	1.005 ± 0.025	0.0251	1.008 ± 0.001	0.451	1.080 ± 0.094

	^{23}Na σ_c		^{55}Mn σ_c		Cu σ_c	
Group	MC^2-2	VIM/MC^2-2	MC^2-2	VIM/MC^2-2	MC^2-2	VIM/MC^2-2
9	0.001709	1.116 ± 0.130	0.01437	1.001 ± 0.001	0.02702	1.000 ± 0.0001
10	0.000223	1.010 ± 0.001	0.02087	1.002 ± 0.002	0.0301	1.000 ± 0.0005
11	0.000292	1.055 ± 0.021	0.02988	0.999 ± 0.004	0.0374	1.000 ± 0.0005
12	0.000272	1.103 ± 0.165	0.0501	1.005 ± 0.007	0.0546	1.001 ± 0.007
13	0.000236	0.993 ± 0.001	0.0766	1.007 ± 0.013	0.0891	1.003 ± 0.016
14	0.000304	0.960 ± 0.001	0.0823	1.001 ± 0.001	0.1474	1.000 ± 0.013
15	0.001448	0.978 ± 0.062	0.0644	1.002 ± 0.009	0.2096	1.010 ± 0.028
16	0.01207	1.000 ± 0.010	0.01239	1.001 ± 0.005	0.2163	1.003 ± 0.021
17	0.1607	0.996 ± 0.008	0.340	1.002 ± 0.006	0.570	0.999 ± 0.032
18	0.01668	0.996 ± 0.003	0.1198	0.997 ± 0.004	0.1126	1.003 ± 0.016
19	0.00902	0.981 ± 0.001	2.057	1.025 ± 0.032	0.0447	1.002 ± 0.0002
20	0.00786	0.992 ± 0.001	0.219	1.000 ± 0.006	3.69	1.019 ± 0.066
21	0.00799	1.000 ± 0.001	1.442	1.008 ± 0.013	0.0438	0.997 ± 0.001
22	0.00838	1.000 ± 0.001	1.099	1.001 ± 0.005	0.504	0.982 ± 0.066

TABLE III. Comparison of Infinite Dilution Broad-Group Unresolved Resonance Cross Sections

	VIM/MC^2-2 (Linear-Linear Interpolation)					
Group	^{238}U σ_c	^{238}U σ_s	Group	^{239}Pu σ_c	^{239}Pu σ_f	^{239}Pu σ_s
11	1.0024 ± 0.0015	1.0008 ± 0.0010	12	0.9995 ± 0.0006	0.9998 ± 0.0002	1.0005 ± 0.0002
12	1.0007 ± 0.0021	1.0002 ± 0.0020	13	0.9991 ± 0.0034	0.9989 ± 0.0020	0.9996 ± 0.0013
13	1.0037 ± 0.0033	1.0037 ± 0.0032	14	0.9967 ± 0.0041	0.9985 ± 0.0026	0.9990 ± 0.0015
14	1.0011 ± 0.0034	0.9996 ± 0.0042	15	0.9993 ± 0.0037	1.0000 ± 0.0023	1.0000 ± 0.0017
15	0.9982 ± 0.0065	0.9995 ± 0.0067	16	1.0009 ± 0.0062	1.0004 ± 0.0042	1.0015 ± 0.0027
16	1.0079 ± 0.0096	1.0040 ± 0.0084	17	1.0025 ± 0.0104	1.0011 ± 0.0053	1.0025 ± 0.0043
			18	0.9958 ± 0.0120	1.0004 ± 0.0088	0.9980 ± 0.0043
			19	1.0087 ± 0.0093	1.0063 ± 0.0072	1.0023 ± 0.0040
			20	0.9976 ± 0.0140	0.9924 ± 0.0113	0.9969 ± 0.0090
			21	0.9836 ± 0.0143	0.9825 ± 0.0100	0.9936 ± 0.0101

significance, while a less restrictive criterion is applied to absorption cross sections to maintain a minimum level of accuracy in cross section representation over the full resonance range.

A number of VIM and ETØE-2/MC^2-2 comparison calculations have been run which illustrate the degree to which agreement has been reached. In these calculations, broad-group edits were produced for 27 groups with a lethargy width of 0.5 from 10 MeV to 13.71 eV. In Table I, broad-group cross sections for ^{238}U capture

TABLE I. Comparison of Infinite Dilution Broad-Group Resonance Cross Sections for Heavy Isotopes

Group	MC^2-2 Integral Transport	VIM/MC^2-2
	^{238}U σ_c	
17	1.419	1.007 ± 0.021
18	1.808	0.997 ± 0.018
19	2.918	0.988 ± 0.024
20	3.67	1.014 ± 0.030
21	3.61	0.981 ± 0.037
22	11.45	1.005 ± 0.030
23	23.6	1.000 ± 0.036
24	25.6	0.980 ± 0.038
25	1.386	1.047 ± 0.017
26	86.8	1.014 ± 0.046
27	126.4	1.042 ± 0.036
	^{239}Pu σ_c	
21	9.87	0.992 ± 0.014
22	14.23	0.998 ± 0.011
23	19.91	1.001 ± 0.019
24	29.5	0.997 ± 0.021
25	58.1	1.003 ± 0.022
26	10.49	0.989 ± 0.021
27	70.6	1.011 ± 0.017
	^{239}Pu σ_f	
21	10.54	0.985 ± 0.010
22	17.03	1.000 ± 0.008
23	19.49	0.997 ± 0.010
24	52.8	1.004 ± 0.013
25	40.0	0.998 ± 0.013
26	11.91	0.995 ± 0.017
27	87.0	1.006 ± 0.012

and ^{239}Pu capture and fission are shown. The problem solved consisted of an infinite homogeneous medium of ^{23}Na with an infinitely dilute admixture of heavy isotopes and a neutron source in the first ultra-fine-group at 10 MeV. The MC^2-2 integral transport option was used. The VIM results are shown with ±2 σ uncertainties. The ^{238}U data set now used by VIM has over 10,000 points in the resolved range; however, the comparison shown in Group 25 indicates some remaining difficulty in interpolation between isolated resonances. Comparable results have been attained with finite concentrations.[3]

Results from the solution of a similar problem, an infinite medium of ^{12}C with infinitely dilute admixtures of structural materials, is shown in Table II. Given a near-perfect energy grid representation in both ETØE-2 and UNIDØP, the UNIDØP thinning procedure together with linear interpolation in VIM should produce slightly higher estimates by VIM for broad-group capture cross sections. Large discrepancies noted in Table II have been traced to energy grid insufficiencies remaining in UNIDØP or ETØE-2. The problem has been reduced for Version 4 data processing by UNIDØP by extending the grid around a resonance out to distance greater than 30,000 times the resonance total width; an alternative would be a denser background grid.

Unresolved Resonance Methods

In comparison of VIM broad-group cross section calculations for unresolved resonances with comparable ETØE-2/MC^2-2 calculations, discrepancies of the order of several percent were frequently observed. The source of these discrepancies was traced largely to numerical limitations in obtaining accurate infinite dilution average cross sections in U3R and to similar limitations in MC^2-2. A high-order quadrature scheme was added to U3R to obtain the dilute averages which are used to normalize the unresolved resonance probability tables; comparable improvements in numerical methods were developed for MC^2-2. Computation of infinite dilution average unresolved resonance cross sections at ENDF/B energy points now shows typical agreement of 0.02% or better.

A more subtle disagreement arises due to differences in interpolation schemes used in the two codes. In VIM, unresolved resonance cross sections at a particular energy during a particular neutron history are chosen by first selecting a probability table by random linear interpolation between table energies; subsequently, cross sections are obtained by random sampling from the selected table. In MC^2-2, unresolved resonance calcuations are made at ENDF/B energy points (which are the same as the energies at which VIM probability tables are specified). Log-log interpolation is then used to produce ultra-fine-group cross sections in the interval. VIM estimates ^{238}U broad-group capture cross sections up to about 1% higher than MC^2-2; capture and fission broad-group cross sections are up to 2% higher in limited regions of the ^{239}Pu unresolved range when estimated by VIM. Examples of this difference are shown in Ref. 3.

The degree to which agreement in unresolved resonance treatment between VIM and MC^2-2 has been achieved, apart from the question of interpolation scheme, was examined by modifying MC^2-2 to perform linear-linear interpolation in the unresolved region. A comparison of results from ^{238}U and ^{239}Pu broad-group unresolved resonance cross sections is shown in Table III; the data are again taken from solutions for slowing down in an infinite medium of ^{23}Na with an infinitely dilute admixture of heavy isotopes. Similar results have been obtained for finite concentrations of the heavy isotopes.

The most direct approach to resolving the interpolation scheme question would be to expand the number of unresolved resonance data points by interpolating unresolved parameters as specified by ENDF/B; the interpolation scheme dependence would thereby be minimized. Increasing the point density is preferable to implementing nonlinear interpolation schemes in VIM, both for running time considerations and for consistency with the probability table method of treating unresolved resonance cross sections.

Nonresonant Cross Section Methods

The conversion of ENDF/B File 3 data to a VIM library file involves the generation of an energy grid, including all essential points of the various reaction types, and the expansion of the reaction cross sections onto the common grid using the appropriate ENDF/B-specified interpolation scheme. The basic method of

grid generation is merely to form the union of the energy grids of all needed reaction types, supplement it with a uniform 20 points per decade mesh, and eliminate any duplicate or nearly duplicate points. Generally, the scheme has been shown to provide a sufficiently dense energy grid so that linear-linear cross section interpolation as performed in VIM provides a highly accurate representation of the original ENDF/B data. However, exceptions have been observed in cases of rapidly fluctuating elastic scattering cross sections such as the iron data in the range 320 keV to 59 keV which requires log-log interpolation.

At the present time, the VIMB3 code has been modified to expand the energy grid describing elastic scattering to sufficient density to ensure that linear-linear interpolation may be done with specified accuracy. Additional grid points are inserted at the location of maximum discrepancy until the interpolation discrepancy nowhere exceeds the input criterion. The expanded grid is then merged with the energy grids from other reaction types as before.

The effect of the improved procedure may be seen in Table IV; the results shown were obtained in the

TABLE IV. Comparison of Iron Broad-Group Scattering Cross Sections

Group	MC^2-2	VIM/MC^2-2[a]	VIM/MC^2-2[b]
7	2.978	0.994 ± 0.004	0.998 ± 0.003
8	3.286	1.009 ± 0.003	1.002 ± 0.004
9	2.943	1.022 ± 0.005	0.997 ± 0.004
10	4.616	1.045 ± 0.004	0.999 ± 0.004
11	4.528	1.001 ± 0.002	1.002 ± 0.002

[a] Previous iron cross section set for VIM.

[b] Current iron cross section set for VIM.

calculations described in Ref. 3. An additional 132 points were required — an increase of less than 3%.

Conclusions

The objective of supplying the VIM code with a faithful representation of ENDF/B Version 3 has, in general, been met. Excellent agreement with ETØE-2/MC^2-2 is being attained in calculations which can be performed by both codes when the more rigorous options of MC^2-2 are used. For those remaining small difficulties which have been noted above, the causes are understood and the remedies are currently being applied in the preparation of the new VIM library generated from ENDF/B Version 4 data.

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Chapter 2

A COMPARISON OF VIM AND MC^2-2 — TWO DETAILED SOLUTIONS OF THE NEUTRON SLOWING-DOWN PROBLEM

A comparison of solutions by the Monte Carlo code VIM and by ETØE-2/MC^2-2 of a zero-dimensional slowing-down problem in the homogeneous ZPR-6 Assembly 7 core composition demonstrates the ability of either code to provide a reliable computational benchmark capability for such calculations.

(Cross section, multigroup, slowing-down, transport, Monte Carlo, resonance, reactor, eigenvalue, benchmark, stochastic)

Introduction

The generation of multigroup cross sections from point data represents one of the basic problems in reactor physics analysis. Since errors introduced into the processed data may lead to a significant uncertainty in the subsequent reactor calculations, there has been a great deal of interest in estimating the error introduced by specific methods and/or codes. In this study two distinct methods are compared for the solution of a zero-dimensional neutron slowing-down problem.[1-3] Both the continuous-energy Monte Carlo code VIM and the multigroup code MC^2-2 were designed to treat such a problem in a rigorous manner. As a consequence, a comparison of the two methods serves to evaluate both methods and codes and verify that they attain a sufficient accuracy in the representation and treatment of neutron interactions to provide a standard for future comparisons.

The problem selected for study was an infinite, homogeneous core composition representative of the benchmark ZPR-6 Assembly 7.[4] The ENDF/B-3 data were used. The atom densities defining the problem are shown in Table I. A uniform temperature of 300°K was used. Broad-group edits were produced for 24 groups with a lethargy width of 0.5 from 10 MeV to 275.36 eV and 1.0 from 275.36 eV to 13.71 eV. Results available for direct comparison included broad-group edits for flux, fission spectrum, isotopic reaction rates, and isotopic microscopic cross sections.

TABLE I. Atom Densities ($\times 10^{-21}$ atoms/cc)

Isotope	ENDF/B Mat No.	Atom Density
^{239}Pu	1159	0.88672
^{240}Pu	1105	0.11944
^{241}Pu	1106	0.0133
^{235}U	1157	0.01259
^{238}U	1158	5.78036
Mo	1111	0.2357
^{23}Na	1156	9.2904
^{16}O	1134	13.98
Fe	1180	12.97
Ni	1123	1.240
Cr	1121	2.709
^{55}Mn	1019	0.212

Features of the VIM Calculation

As a continuous-energy Monte Carlo code, VIM provides a detailed energy and angular representation of neutron physics data obtained from ENDF/B libraries. Outside of the unresolved resonance region, isotopic microscopic cross sections are obtained by linear interpolation from dense cross section versus energy tables (Doppler broadened to 300°K in the resolved region). In an unresolved resonance region, cross sections are obtained by random sampling from probability tables corresponding to each ENDF/B specified unresolved resonance data point. Probability distributions are employed to represent anisotropy in the center of mass for both discrete level inelastic and elastic scattering. The full ENDF/B energy dependence of parameters for the determination of the energy distribution of secondary neutrons is utilized in VIM.

Of the 12 isotopes in the problem, 8 had new cross section sets prepared as described in Ref. 1: ^{238}U, ^{239}Pu, ^{240}Pu, Ni, Cr, Fe, ^{23}Na, and ^{55}Mn. A second iron cross section set was prepared, incorporating some small additional refinements, and used in a second VIM calculation.

The first VIM calculation, designated as VIM Run No. 1, consisted of 25,000 neutron histories. Absorption weighting was used to produce low variance estimates of reaction rates down to very low energies. A second VIM calculation, designated as VIM Run No. 2, consisted of 50,000 neutron histories followed with analog weighting. The iron cross section set used in the second run resulted in lower iron scattering cross sections, about 5% or less, from 320 keV to 59 keV. The results of both runs are presented below for quantities significantly affected by the change in iron scattering.

Eigenvalue estimation in VIM is made simultaneously with analog, collision, and track length estimators. Simple averaging of these estimators is used to reduce variance as is the method of combined estimators.[5] The detailed edits of isotopic reaction rates by energy group and group fluxes are obtained by track length estimation.

Features of the ETØE-2/MC^2-2 Calculation

The MC^2-2 code[6] solves the fundamental mode neutron slowing-down equations using multigroup, continuous slowing-down, and integral transport theory algorithms. The input data to MC^2-2 are prepared by the code ETØE-2 which reformats and preprocesses data from the ENDF/B tapes. The formats required by MC^2-2 were specified to permit efficient access to data by a processing code and thus are less general than the ENDF/B formats. The reformatting done by ETØE-2 does not, however, change the basic physics data. On the other hand, the processing of floor cross section data and light-element resonance data by ETØE-2 to ultra-fine-group cross sections ($\Delta u \approx 1/120$) does introduce approximations. In the initial comparisons of VIM and MC^2-2, many of the differences were traced to an inadequate treatment of the light-element resonances by ETØE-2. The numerical algoriths were refined as a consequence of this testing. The MC^2-2 code uses these data to calculate a flux and current spectrum which are used to collapse the data to broad-group cross sections

The rigor of the slowing-down calculation is user-specified. The comparison calculations reported in this study were performed using most of the more rigorous algorithms. In particular, isotope-dependent fission spectra, improved Goertzel-Greuling moderating parameters, detailed elastic matrix, and resonance calculations were used in the ultra-fine-group calculation and a hyperfine-group integral transport calculation was used below 4 keV to treat the resolved resonance region in detail. It has been found that one may relax the rigor of the calculation without much impact on such integral parameters as k_{eff}, whereas group cross section or flux comparisons require the most rigorous methods.

Results

Extremely close agreement in the eigenvalue computation was obtained. The ETØE-2/MC^2-2 value of 1.2121 is well within one standard deviation of both the VIM Run No. 1 value of 1.2128 (1 σ = 0.0014) and the VIM Run No. 2 value of 1.2129 (1 σ = 0.0030).

A comparison of group flux calculations is shown in Table II; the VIM results are shown with uncertainties of ±2 σ. The effect of the improvement in iron scattering cross sections used in VIM Run No. 2 may be noted in the data for Groups 8, 9, and 10. Although generally good agreement is obtained over the full energy range, the VIM spectrum appears slightly harder. A slightly more rapid attenuation is apparent in the VIM-computed flux below Group 16. It should be noted that the observed agreement in low-energy flux is attainable only with the MC^2-2 integral transport option.

TABLE II. Group Flux Comparison

Group No.	MC^2-2	VIM Run No. 1 MC^2-2	VIM Run No. 2 MC^2-2
1	0.4800	1.048 ± 0.106	0.977 ± 0.072
2	1.989	1.016 ± 0.060	1.048 ± 0.034
3	4.904	1.006 ± 0.034	1.010 ± 0.022
4	7.335	0.995 ± 0.026	0.993 ± 0.017
5	8.868	1.009 ± 0.022	1.002 ± 0.016
6	17.40	1.018 ± 0.015	0.997 ± 0.009
7	17.10	1.009 ± 0.011	1.005 ± 0.011
8	22.13	0.991 ± 0.010	1.002 ± 0.009
9	24.22	0.991 ± 0.008	1.005 ± 0.008
10	21.54	0.994 ± 0.008	1.000 ± 0.009
11	18.50	0.998 ± 0.008	0.999 ± 0.009
12	14.62	1.007 ± 0.007	1.005 ± 0.011
13	15.10	0.994 ± 0.008	1.006 ± 0.009
14	11.19	0.997 ± 0.008	0.999 ± 0.014
15	6.252	0.998 ± 0.006	1.006 ± 0.015
16	3.937	0.995 ± 0.007	0.992 ± 0.017
17	1.428	0.994 ± 0.010	0.999 ± 0.020
18	4.249	0.991 ± 0.009	1.000 ± 0.022
19	2.800	0.989 ± 0.010	1.011 ± 0.026
20	1.555	0.987 ± 0.014	0.989 ± 0.038
21	0.6586	0.977 ± 0.019	0.982 ± 0.048
22	0.4096	0.970 ± 0.034	0.963 ± 0.084
23	0.02851	0.951 ± 0.066	0.982 ± 0.258
24	0.000719	0.797 ± 0.260	1.248 (1 σ = ±0.678)

Individual isotopic capture rates are shown in Table III and fission rates in Table IV. The MC^2-2 rates shown were obtained without benefit of the integral transport option. The VIM results are again shown with ±2 σ uncertainties. The discrepancy in ^{238}U capture rate results primarily from the difference between the VIM and the MC^2-2 unresolved resonance treatment as will be discussed below. The very significant difference in iron capture is localized in Group 19 and undoubtedly results from the difference in the treatment of self-shielding of the 1150-eV p-wave resonance. In the VIM data library, approximately 40 points are used to represent this resonance, whereas in the ETØE-2 library, its strength is almost totally confined to one ultrafine group. Apart from the exceptions noted here, however, the agreement in reaction rates is generally good.

TABLE III. Isotopic Capture Rates

Isotope	MC^2-2	VIM Run No. 1 MC^2-2	VIM Run No. 2 MC^2-2
^{240}Pu	0.012385	0.9943 ± 0.0061	0.9998 ± 0.0126
^{241}Pu	0.0014452	0.9998 ± 0.0047	1.0047 ± 0.0103
^{235}U	0.0017975	0.9925 ± 0.0042	0.9992 ± 0.0101
^{238}U	0.3858	1.0052 ± 0.0038	1.0119 ± 0.0096
^{239}Pu	0.11419	0.9947 ± 0.0050	1.0029 ± 0.0122
Cr	0.011056	0.9853 ± 0.0132	0.9994 ± 0.0266
Ni	0.008198	1.0054 ± 0.0084	1.0072 ± 0.0114
Fe	0.03055	0.9704 ± 0.0142	0.9745 ± 0.0302
^{23}Na	0.004485	0.9921 ± 0.0104	1.0087 ± 0.0168
^{16}O	0.0019893	1.0354 ± 0.0574	1.0127 ± 0.0348
Mo	0.008655	0.9935 ± 0.0057	1.0040 ± 0.0148
^{55}Mn	0.003685	1.0062 ± 0.0126	1.0193 ± 0.0294

TABLE IV. Isotopic Fission Rates

Isotope	MC^2-2	VIM Run No. 1 MC^2-2	VIM Run No. 2 MC^2-2
^{240}Pu	0.007857	1.0000 ± 0.0094	1.0043 ± 0.0074
^{241}Pu	0.007516	0.9991 ± 0.0034	1.0020 ± 0.0078
^{235}U	0.005712	0.9946 ± 0.0031	0.9998 ± 0.0080
^{238}U	0.04288	1.0030 ± 0.0210	1.0077 ± 0.0141
^{239}Pu	0.3523	0.9972 ± 0.0033	1.0037 ± 0.0065

A detailed comparison of broad-group cross sections for ^{238}U capture and ^{239}Pu capture and fission below 40.9 keV are given in Table V. The very close agreement in the resolved range was obtained through use of the MC^2-2 integral transport option. The VIM results are shown with ±2 σ uncertainties.

Although broad-group cross section agreement as shown is typically of the order of 1% and frequently better, an important difference may be noted in the ^{238}U unresolved resonance range. The VIM code uses random linear-linear cross-section interpolation between probability tables generated for ENDF/B unresolved resonance energy points; MC^2-2 uses log-log interpolation between unresolved resonance calculations at specified energies. It has been determined that the difference in interpolation schemes alone will account for the greater part of the 0.5% to 1.0% increase in the VIM estimate of ^{238}U unresolved resonance capture over the corresponding MC^2-2 results.[3] Similar effects may be noted in ^{239}Pu fission, particularly in Group 18 where the difference in interpolation scheme produces a 2% greater VIM result.

In Table VI, a comparison of capture cross sections for structural materials over the energy range 820.9 keV to 748.5 eV is shown. The examples shown represent what are perhaps the most difficult cases in which to attain close agreement. The VIM data presented are shown with ±2 σ uncertainties and were taken from VIM Run No. 2 for Groups 6 to 15 and from VIM Run No. 1 for Groups 16 to 19. Although the agreement is frequently very good, a number of significant exceptions

TABLE V. Detailed Broad-Group Cross-Section Comparison

Group No.	$^{238}U\ \sigma_c$		$^{239}Pu\ \sigma_c$		$^{239}Pu\ \sigma_f$	
	MC²-2	VIM/MC²-2	MC²-2	VIM/MC²-2	MC²-2	VIM/MC²-2
12	0.4331	1.006 ± 0.002	0.5574	0.998 ± 0.001	1.7410	0.999 ± 0.0003
13	0.5290	1.011 ± 0.003	0.7706	1.001 ± 0.003	1.7679	1.000 ± 0.002
14	0.6408	1.006 ± 0.003	1.0587	1.001 ± 0.004	1.9175	1.000 ± 0.002
15	0.7622	1.008 ± 0.005	1.5853	1.006 ± 0.005	2.171	1.001 ± 0.003
16	0.8728	0.999 ± 0.008	2.156	1.004 ± 0.005	2.496	1.003 ± 0.004
17	1.1485	0.999 ± 0.018	3.387	1.006 ± 0.009	2.846	1.006 ± 0.006
18	1.0126	1.012 ± 0.013	3.496	1.011 ± 0.007	4.204	1.020 ± 0.005
19	1.3022	1.010 ± 0.018	4.283	1.006 ± 0.009	5.789	1.007 ± 0.006
20	1.3559	1.006 ± 0.025	6.332	1.001 ± 0.013	8.144	1.011 ± 0.009
21	1.3596	1.010 ± 0.033	7.349	1.016 ± 0.020	9.486	1.008 ± 0.012
22	1.9684	1.014 ± 0.027	12.645	1.006 ± 0.017	15.728	1.012 ± 0.012
23	1.9908	1.078 ± 0.088	14.849	0.979 ± 0.046	36.00	0.993 ± 0.033
24	8.467	0.989 ± 0.220	10.819	1.055 ± 0.216	13.79	0.978 ± 0.184

TABLE VI. Detailed Broad-Group Cross-Section Comparison

Group No.	Cr σ_γ		Ni σ_γ		Fe σ_γ	
	MC²-2	VIM/MC²-2	MC²-2	VIM/MC²-2	MC²-2	VIM/MC²-2
6	0.003873	1.072 ± 0.003	0.007570	1.006 ± 0.001	0.005150	1.0000 ± 0.0002
7	0.003939	0.998 ± 0.005	0.007989	1.008 ± 0.003	0.004997	1.0000 ± 0.0001
8	0.003909	0.973 ± 0.013	0.009657	1.004 ± 0.003	0.006100	1.0003 ± 0.0011
9	0.006492	0.993 ± 0.020	0.01425	1.000 ± 0.003	0.005498	1.0002 ± 0.0003
10	0.009700	1.011 ± 0.011	0.01701	1.003 ± 0.004	0.008763	0.9999 ± 0.0002
11	0.01503	0.991 ± 0.032	0.02375	0.997 ± 0.030	0.006547	1.035 ± 0.044
12	0.02932	1.009 ± 0.014	0.03816	1.006 ± 0.041	0.01691	1.014 ± 0.047
13	0.03423	1.042 ± 0.038	0.05977	0.995 ± 0.020	0.005640	0.987 ± 0.114
14	0.03149	1.001 ± 0.005	0.1039	0.998 ± 0.029	0.009607	0.984 ± 0.053
15	0.08302	0.999 ± 0.004	0.02020	1.029 ± 0.027	0.02631	0.999 ± 0.007
16	0.06855	1.002 ± 0.002	0.03647	1.002 ± 0.016	0.007592	1.004 ± 0.006
17	0.02341	1.001 ± 0.001	0.06266	1.129 ± 0.059	0.005840	1.013 ± 0.012
18	0.2108	0.897 ± 0.056	0.02242	1.004 ± 0.005	0.01086	1.071 ± 0.018
19	0.01974	1.005 ± 0.001	0.02494	1.007 ± 0.001	0.2546	0.930 ± 0.038

may be noted. Two major causes contribute to the differences:

(1) insufficient point densities in the VIM library in the extreme wings of narrow resonances may cause a bias toward higher capture in the valleys between isolated narrow resonances; and

(2) the much less detailed treatment of the peaks of very narrow capture resonances in ETØE-2 causes higher ETØE-2/MC²-2 cross sections by underestimating self-shielding of the narrow resonances.

The latter effect is most noticeable in iron in Group 19, due to the 1150-eV resonance, and in chromium in Group 18, due to the 1626-eV resonance. The former difficulty probably accounts for the chromium discrepancy in Group 6 and in nickel in Group 18. A combination of these effects probably contributes to a lesser extent in other cases.

A comparison of other broad-group cross section data shows that agreement in total cross sections is generally within a few tenths of 1% and within 1% on capture throughout the resonance regions of the various isotopes. Other examples of the above difficulties with narrow capture resonances may be detected. The interpolation difficulty in the unresolved region described above appears to have little effect for ^{240}Pu, ^{241}Pu, or ^{235}U. Following the preparation of an improved iron data set for the VIM library, providing improved interpolation accuracy above the resonance region, no significant disagreement is observed with respect to nonresonant cross sections.

Conclusions

In recent years several studies have been reported which compare neutron cross section processing methods and codes. Such studies have generally concentrated on comparison of k_{eff} and reaction rate ratios and concluded that the methods and codes were in good agreement if k_{eff} differences were less than 0.5%. The current study was designed to determine whether there was agreement on a range of parameters between an essentially exact stochastic calculation and a detailed analytic calculation for a typical fast reactor core mixture. The extremely good agreement between the two methods permits one to conclude that either code provides a reliable computational benchmark capability for such an infinite medium calculation.

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